



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2024 – 10:11 AM JST

PDB ID : 8ZD5
Title : Crystal structure of E40K variant of Cu/Zn-superoxide dismutase from dog (Canis familiaris) in the holo form complexed with 22E1 Fv-clasp
Authors : Shino, Y.; Furukawa, Y.; Muraki, N.
Deposited on : 2024-05-01
Resolution : 2.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

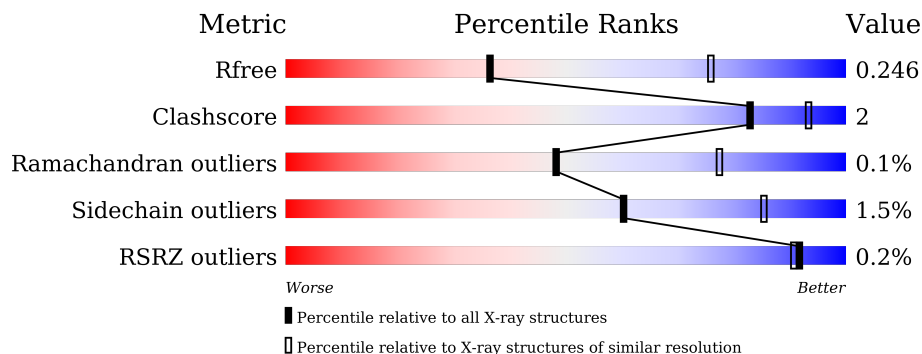
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	169	93% 5% ..
1	E	169	89% 8% ..
1	H	169	92% 6% .
1	K	169	86% 7% 7%
2	C	159	84% 10% 6%
2	F	159	85% 9% . 6%

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Mol	Chain	Length	Quality of chain
2	I	159	 <p>% 86% 11%</p>
2	L	159	 <p>85% 6% 9%</p>
3	A	153	 <p>93% 7%</p>
3	D	153	 <p>93% 6%</p>
3	G	153	 <p>94% 5%</p>
3	J	153	 <p>93% 6%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14154 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 22E1VH-SARAH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	166	1299	821	210	261	7	0	0	0
1	E	164	1295	820	210	258	7	0	0	0
1	B	167	1283	805	212	260	6	0	0	0
1	K	157	1246	787	203	249	7	0	0	0

- Molecule 2 is a protein called 22E1VL-SARAH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	150	1174	733	199	236	6	0	0	0
2	C	150	1177	736	199	236	6	0	0	0
2	L	145	1136	713	191	227	5	0	0	0
2	I	142	1106	695	185	220	6	0	0	0

- Molecule 3 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	153	1106	679	203	218	6	0	0	0
3	D	153	1106	679	203	218	6	0	0	0
3	G	153	1109	680	203	220	6	0	0	0
3	J	153	1109	680	203	220	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	LYS	GLU	engineered mutation	UNP Q8WNN6
A	51	GLY	GLU	conflict	UNP Q8WNN6
A	53	ASN	UNK	conflict	UNP Q8WNN6
D	40	LYS	GLU	engineered mutation	UNP Q8WNN6
D	51	GLY	GLU	conflict	UNP Q8WNN6
D	53	ASN	UNK	conflict	UNP Q8WNN6
G	40	LYS	GLU	engineered mutation	UNP Q8WNN6
G	51	GLY	GLU	conflict	UNP Q8WNN6
G	53	ASN	UNK	conflict	UNP Q8WNN6
J	40	LYS	GLU	engineered mutation	UNP Q8WNN6
J	51	GLY	GLU	conflict	UNP Q8WNN6
J	53	ASN	UNK	conflict	UNP Q8WNN6

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

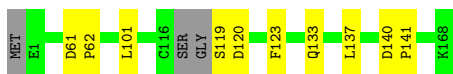
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cu 1 1	0	0
5	D	1	Total Cu 1 1	0	0
5	G	1	Total Cu 1 1	0	0
5	J	1	Total Cu 1 1	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

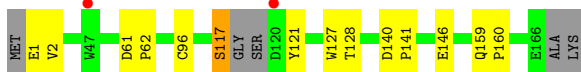
- Molecule 1: 22E1VH-SARAH

Chain H:  92% 6% .

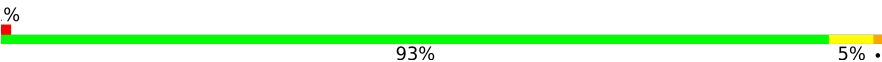


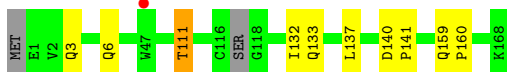
- Molecule 1: 22E1VH-SARAH

Chain E:  89% 8% ..




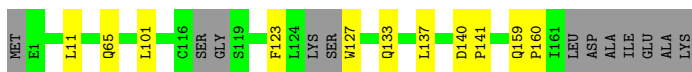
- Molecule 1: 22E1VH-SARAH

Chain B:  93% 5% ..




- Molecule 1: 22E1VH-SARAH

Chain K:  86% 7% 7%




- Molecule 2: 22E1VL-SARAH

Chain F:  85% 9% . 6%

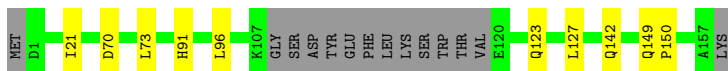
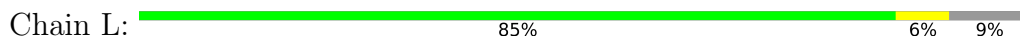


- Molecule 2: 22E1VL-SARAH

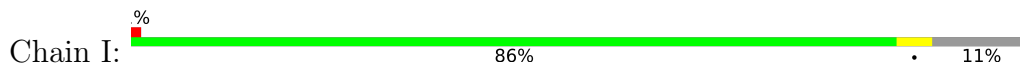
Chain C:  84% 10% 6%



- Molecule 2: 22E1VL-SARAH



- Molecule 2: 22E1VL-SARAH



- Molecule 3: Superoxide dismutase [Cu-Zn]



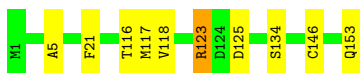
- Molecule 3: Superoxide dismutase [Cu-Zn]



- Molecule 3: Superoxide dismutase [Cu-Zn]



- Molecule 3: Superoxide dismutase [Cu-Zn]



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.91Å 82.21Å 187.61Å 90.00° 108.46° 90.00°	Depositor
Resolution (Å)	48.15 – 2.89 48.15 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.15-2.89) 97.8 (48.15-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.201 , 0.249 0.204 , 0.246	Depositor DCC
R_{free} test set	2716 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtrriage
Anisotropy	0.371	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14154	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.34	0/1308	0.59	0/1775
1	E	0.35	0/1324	0.62	0/1796
1	H	0.30	0/1327	0.57	0/1800
1	K	0.34	0/1273	0.60	0/1724
2	C	0.36	0/1199	0.68	0/1622
2	F	0.35	0/1194	0.67	0/1613
2	I	0.34	0/1126	0.64	0/1521
2	L	0.32	0/1156	0.59	0/1562
3	A	0.35	0/1123	0.59	0/1512
3	D	0.36	0/1123	0.60	0/1512
3	G	0.33	0/1126	0.57	0/1516
3	J	0.33	0/1126	0.61	0/1516
All	All	0.34	0/14405	0.61	0/19469

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	I	0	1
3	A	0	1
3	D	0	1
3	J	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	123	ARG	Sidechain
3	D	123	ARG	Sidechain
2	F	53	ARG	Sidechain
2	I	53	ARG	Sidechain
3	J	123	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1283	0	1199	6	0
1	E	1295	0	1220	7	0
1	H	1299	0	1221	5	0
1	K	1246	0	1174	7	0
2	C	1177	0	1140	8	0
2	F	1174	0	1150	9	0
2	I	1106	0	1089	2	0
2	L	1136	0	1110	5	0
3	A	1106	0	1088	6	0
3	D	1106	0	1088	6	0
3	G	1109	0	1090	5	0
3	J	1109	0	1090	5	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
All	All	14154	0	13659	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:NE2	1:B:111:THR:HG22	2.11	0.66
1:B:6:GLN:HE21	1:B:111:THR:HG22	1.61	0.65
1:K:123:PHE:O	1:K:127:TRP:CD1	2.53	0.62
1:H:120:ASP:O	1:H:123:PHE:HB3	2.00	0.61
2:F:39:LYS:HB3	2:F:40:PRO:HD2	1.83	0.61

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/169 (96%)	158 (97%)	5 (3%)	0	100	100
1	E	160/169 (95%)	156 (98%)	4 (2%)	0	100	100
1	H	162/169 (96%)	157 (97%)	5 (3%)	0	100	100
1	K	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
2	C	146/159 (92%)	144 (99%)	2 (1%)	0	100	100
2	F	146/159 (92%)	142 (97%)	3 (2%)	1 (1%)	19	49
2	I	138/159 (87%)	135 (98%)	3 (2%)	0	100	100
2	L	141/159 (89%)	139 (99%)	2 (1%)	0	100	100
3	A	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
3	D	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
3	G	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
3	J	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
All	All	1811/1924 (94%)	1763 (97%)	47 (3%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	40	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	133/146 (91%)	131 (98%)	2 (2%)	60	85
1	E	137/146 (94%)	133 (97%)	4 (3%)	37	72
1	H	136/146 (93%)	135 (99%)	1 (1%)	81	94
1	K	133/146 (91%)	133 (100%)	0	100	100
2	C	128/142 (90%)	127 (99%)	1 (1%)	79	93
2	F	129/142 (91%)	125 (97%)	4 (3%)	35	70
2	I	121/142 (85%)	120 (99%)	1 (1%)	79	93
2	L	123/142 (87%)	122 (99%)	1 (1%)	79	93
3	A	118/119 (99%)	116 (98%)	2 (2%)	56	83
3	D	118/119 (99%)	116 (98%)	2 (2%)	56	83
3	G	119/119 (100%)	117 (98%)	2 (2%)	56	83
3	J	119/119 (100%)	117 (98%)	2 (2%)	56	83
All	All	1514/1628 (93%)	1492 (98%)	22 (2%)	60	85

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	130	ASP
1	B	3	GLN
3	J	134	SER
1	B	111	THR
1	E	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	149	GLN
2	I	69	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	167/169 (98%)	-0.49	1 (0%) 85 82	57, 88, 161, 189	0
1	E	164/169 (97%)	-0.49	2 (1%) 76 71	53, 79, 147, 186	0
1	H	166/169 (98%)	-0.14	0 100 100	75, 121, 167, 209	0
1	K	157/169 (92%)	-0.36	0 100 100	61, 85, 174, 207	0
2	C	150/159 (94%)	-0.53	0 100 100	54, 92, 135, 178	0
2	F	150/159 (94%)	-0.55	0 100 100	52, 89, 132, 165	0
2	I	142/159 (89%)	-0.39	1 (0%) 84 80	64, 97, 140, 172	0
2	L	145/159 (91%)	-0.41	0 100 100	68, 105, 177, 210	0
3	A	153/153 (100%)	-0.58	0 100 100	59, 84, 124, 156	0
3	D	153/153 (100%)	-0.68	0 100 100	55, 74, 111, 172	0
3	G	153/153 (100%)	-0.37	0 100 100	81, 110, 158, 183	0
3	J	153/153 (100%)	-0.45	0 100 100	75, 104, 141, 172	0
All	All	1853/1924 (96%)	-0.45	4 (0%) 92 91	52, 96, 158, 210	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	120	ASP	3.9
1	B	47	TRP	3.9
1	E	47	TRP	2.2
2	I	4	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CU	G	202	1/1	0.98	0.03	114,114,114,114	0
5	CU	J	202	1/1	0.98	0.03	104,104,104,104	0
5	CU	D	202	1/1	0.99	0.03	78,78,78,78	0
4	ZN	G	201	1/1	0.99	0.03	118,118,118,118	0
4	ZN	J	201	1/1	0.99	0.05	101,101,101,101	0
4	ZN	A	201	1/1	1.00	0.03	82,82,82,82	0
4	ZN	D	201	1/1	1.00	0.02	67,67,67,67	0
5	CU	A	202	1/1	1.00	0.03	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.